Versatile coordination of cyclopentadienyl-arene ligands and its role in titanium-catalyzed ethylene trimerization

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'JACS'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2009-02-09  09:05:58

 Consider this CIF submission for deposition of the second
 X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : q1083)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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# 3. TITLE AND AUTHOR LIST

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# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


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_publ_author_name
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'?' # author name
;   # author related footnote
;
;   # Address of this author
;
   'Meetsma, Auke'
;
 ? # author related footnote
;
;
```

```
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#===============================================================================

# 4. TEXT

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;
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;
 Derived values do not contain the contribution of the distorted-
  and squeezed solvate molecules.

The scattering power of the crystals investigated was very weak:
  nearby an half of the unique (till \q = 25.02 \%), merged reflections
  obey the Fo * 4.0 *(Fo) criterion of observability.
 This implies that the mean s.u. is large compared to the mean magnitude
  of the (even more than double of the squared) structure factor.
 The weak scattering power might be the result of a disorder problem.

The asymmetric unit consists of three moieties: a cationic Ti-complex,
  a fluorinated-tetraphenylborate anion, and  an half highly disordered
  bromobenzene solvate molecule.

The structure was solved by Patterson methods and extension of the
  model was accomplished by direct methods applied to difference
  structure factors using the program DIRDIF7 The positional and
  anisotropic displacement parameters for the non-hydrogen atoms
  were refined. From the solution, it was clear the bromobenzene solvate
  molecule was highly disordered over an inversion center: no satisfactory
  discrete model could be fitted in this density. The BYPASS (SQUEEZE)
  procedure was used to take into account the electron density in the
  potential solvent area of 570.4 \%A^3^/unit cell).

Refinement was further frustrated by an other disorder problem: some
  atoms of the Cp- and phenyl-rings positions were disordered:
  the electron density of the atoms appeared to be spread out.
 The disorder in the rings suggested an interchange of the rings.
 The disorder phenomena may account for the observed unrealistic
  displacement parameters for some atoms when allowed to vary
  anisotropically, as a consequence of the disorder.
```

This is in line with the weak scattering power of the crystals investigated.

To improve the parameters more reasonable, ultimately restrain instructions (DELU, SIMU) for the C-atoms were applied in the refinement.

The hydrogen atoms were generated by geometrical considerations, constrained to idealized geometries, and allowed to ride on the carrier atom with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms, with U~iso~(H) = 1.2U~eq~(C) or 1.5U~eq~(methyl C). The methyl-groups were refined as rigid groups, which were allowed to rotate freely. Assigned values of bond distances: methyl C-H~3~ = 0.98 \%A and aromatic C-H = 0.95 \%A.
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_publ_section_related_literature
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Insert blank lines between references

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Allen, F.H. (2002). Acta Cryst. B58, 380-388.

Beurskens, P.T., Beurskens, G., Gelder, R. de, Smits, J.M.M., Garc\'ia-Granda, S. & Gould, R.O. (2008). The DIRDIF08 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

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Hahn, T. (1983). Ed. International Tables for Crystallography, Volume A, Space-group symmetry, Kluwer Academic Publishers, Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2008). Extended version of the program PLUTO. University of Groningen, The Netherlands. (unpublished).

Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.

Wilson, A.J.C. (1992). Ed. International Tables for Crystallography, Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.
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Fig. 1. Perspective PLUTO drawings of the molecule illustrating the configuration and the adopted numbering scheme.

```
   Fig. 2. Molecular packing viewed down unit cell axes.

   Fig. 3. Perspective ORTEP drawings of the title compound.
           Displacement ellipsoids for non-H atoms are represented at the 50%
           probability level.
           The H-atoms have been omitted to improve clarity.
;

_publ_section_acknowledgements
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# 5. CHEMICAL DATA

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;
;
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_chemical_melting_point              ?
_chemical_formula_moiety
'C24 B F20, C16 H21 Ti'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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'C40 H21 B F20 Ti'
_chemical_formula_iupac              ?
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loop_
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Ti  Ti    0.2776    0.4457
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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# 6. CRYSTAL DATA

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_symmetry_Int_Tables_number                14

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
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   1 x,y,z
   2 -x,1/2+y,1/2-z
   3 -x,-y,-z
   4 x,1/2-y,1/2+z

_cell_length_a                         10.791(1)
_cell_length_b                         13.320(1)
_cell_length_c                         28.398(3)
_cell_angle_alpha                      90
_cell_angle_beta                       91.066(2)
_cell_angle_gamma                      90
_cell_volume                          4081.1(7)
_cell_formula_units_Z                 4

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      9603
_cell_measurement_theta_min        2.35
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_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   9603 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'platelet'
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_exptl_crystal_density_meas       ?
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_exptl_crystal_F_000              1872
_exptl_absorpt_coefficient_mu     0.33
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_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
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_diffrn_radiation_detector
;
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;
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;
  Bruker Smart Apex; CCD area detector
;
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_diffrn_measurement_method           '\f and \w scans'
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;
 Crystal into the cold nitrogen stream of the low-temparature unit
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;
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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_av_sigmaI/netI      0.0977
_diffrn_reflns_limit_h_min         -12
_diffrn_reflns_limit_h_max         12
_diffrn_reflns_limit_k_min         -15
_diffrn_reflns_limit_k_max         15
_diffrn_reflns_limit_l_min         -33
_diffrn_reflns_limit_l_max         33
_diffrn_reflns_theta_min           2.39
_diffrn_reflns_theta_max           25.03
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_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
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 DIRDIF-08 (Beurskens et al., 2008)
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_computing_structure_refinement      'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
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 PLATON (Spek, 2003)
 PLUTO (Meetsma, 2008)
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_computing_publication_material      'PLATON (Spek, 2003)'

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# 8. REFINEMENT DATA


_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type           full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
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_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  '.'

_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         7155
_refine_ls_number_parameters     563
_refine_ls_number_restraints     640
_refine_ls_number_constraints    ?
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_refine_ls_R_factor_gt           0.0707
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_refine_ls_wR_factor_gt          0.1726
_refine_ls_goodness_of_fit_ref   1.041
_refine_ls_restrained_S_all      1.028
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C12 C Uani -0.0742(6) 0.1869(5) 0.1179(2) 1.000 0.053(2) . .
C13 C Uani -0.1243(8) 0.1052(7) 0.1240(3) 1.000 0.075(3) . .
C14 C Uani -0.0634(6) 0.0258(5) 0.1285(3) 1.000 0.058(2) . .
C15 C Uani 0.0565(5) 0.0213(4) 0.1206(2) 1.000 0.0385(17) . .
C16 C Uani 0.1231(5) 0.1100(3) 0.10961(17) 1.000 0.0244(14) . .
C17 C Uani 0.2652(5) 0.1166(3) 0.11405(19) 1.000 0.0273(14) . .
C18 C Uani 0.3309(6) 0.0197(4) 0.0996(2) 1.000 0.045(2) . .
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C111 C Uani 0.2491(5) 0.2294(4) 0.1884(2) 1.000 0.0325(17) . .
C112 C Uani 0.2250(6) 0.2205(6) 0.2360(3) 1.000 0.064(2) . .
C113 C Uani 0.2316(5) 0.1069(7) 0.2482(2) 1.000 0.073(2) . .
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C115 C Uani -0.0486(5) 0.2494(4) 0.2192(2) 1.000 0.0367(17) . .
C116 C Uani -0.0205(5) 0.0159(4) 0.2313(2) 1.000 0.0413(19) . .


H11 H Uiso 0.08344 0.26060 0.10325 1.000 0.0341 . .
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H13 H Uiso -0.21211 0.10230 0.12543 1.000 0.0899 . .
H14 H Uiso -0.10511 -0.03347 0.13790 1.000 0.0700 . .
H15 H Uiso 0.09838 -0.04135 0.12227 1.000 0.0462 . .
H18 H Uiso 0.30613 0.00209 0.06729 1.000 0.0674 . .
H18' H Uiso 0.30779 -0.03469 0.12094 1.000 0.0674 . .
H18" H Uiso 0.42083 0.02986 0.10137 1.000 0.0674 . .
H19 H Uiso 0.40969 0.20182 0.08814 1.000 0.0545 . .
H19' H Uiso 0.28738 0.26676 0.09670 1.000 0.0545 . .
H19" H Uiso 0.29467 0.19421 0.05192 1.000 0.0545 . .
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F22 F Uani 0.1935(2) 0.78631(18) 0.15155(10) 1.000 0.0243(9) . .
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F24 F Uani -0.1722(2) 0.5985(2) 0.13259(11) 1.000 0.0358(10) . .
F25 F Uani -0.0348(2) 0.43019(19) 0.11760(10) 1.000 0.0288(9) . .
F26 F Uani 0.2086(2) 0.43632(17) 0.11843(9) 1.000 0.0201(8) . .
F28 F Uani 0.3338(3) 0.53137(19) 0.04748(9) 1.000 0.0268(9) . .
F29 F Uani 0.4650(3) 0.3825(2) 0.00992(11) 1.000 0.0371(11) . .
F210 F Uani 0.6641(3) 0.3026(2) 0.05829(12) 1.000 0.0440(11) . .
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F216 F Uani 0.4241(3) 0.6572(2) 0.34351(10) 1.000 0.0383(11) . .
F217 F Uani 0.4700(3) 0.8220(2) 0.28882(11) 1.000 0.0403(11) . .
F218 F Uani 0.4359(3) 0.81579(18) 0.19684(10) 1.000 0.0280(10) . .
F220 F Uani 0.6136(2) 0.7128(2) 0.15171(11) 1.000 0.0339(10) . .
F221 F Uani 0.7225(3) 0.8513(2) 0.09861(14) 1.000 0.0568(13) . .
F222 F Uani 0.6021(3) 0.9267(2) 0.02096(13) 1.000 0.0548(14) . .
F223 F Uani 0.3657(3) 0.8653(2) 0.00005(11) 1.000 0.0476(13) . .
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C24 C Uani -0.0471(4) 0.6039(3) 0.13292(18) 1.000 0.0230(14) . .
C25 C Uani 0.0223(4) 0.5190(3) 0.12560(17) 1.000 0.0217(14) . .
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C27 C Uani 0.4494(4) 0.5287(3) 0.11910(17) 1.000 0.0199(14) . .
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C219 C Uani 0.4253(4) 0.7177(3) 0.10680(17) 1.000 0.0209(14) . .
C220 C Uani 0.5460(4) 0.7503(3) 0.1149(2) 1.000 0.0262(14) . .
C221 C Uani 0.6065(5) 0.8204(4) 0.0873(2) 1.000 0.0351(19) . .
C222 C Uani 0.5454(5) 0.8580(4) 0.0480(2) 1.000 0.0334(17) . .
C223 C Uani 0.4278(5) 0.8278(3) 0.03779(19) 1.000 0.0305(16) . .
C224 C Uani 0.3691(5) 0.7596(3) 0.06730(18) 1.000 0.0256(16) . .
B2 B Uani 0.3681(5) 0.6257(4) 0.1392(2) 1.000 0.0180(14) . .


loop_
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_atom_site_aniso_U_33
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_atom_site_aniso_U_13
_atom_site_aniso_U_12
F22 0.0222(14) 0.0133(13) 0.0374(18) -0.0031(12) -0.0009(12) 0.0008(11)
F23 0.0226(15) 0.0200(14) 0.053(2) -0.0027(14) 0.0011(14) 0.0083(12)
F24 0.0126(14) 0.0339(17) 0.061(2) -0.0010(15) 0.0010(14) 0.0037(12)
F25 0.0197(14) 0.0204(15) 0.0463(19) 0.0011(13) 0.0005(13) -0.0052(11)
F26 0.0192(13) 0.0132(13) 0.0281(16) -0.0034(11) 0.0036(11) -0.0003(10)
F28 0.0320(16) 0.0211(15) 0.0274(17) -0.0014(12) 0.0042(13) 0.0000(12)
F29 0.054(2) 0.0248(16) 0.0333(19) -0.0069(14) 0.0197(15) 0.0011(14)
F210 0.0437(19) 0.0293(18) 0.060(2) -0.0120(16) 0.0248(17) 0.0126(14)
F211 0.0174(14) 0.0259(16) 0.065(2) 0.0049(15) 0.0070(14) 0.0090(12)
F212 0.0129(13) 0.0215(14) 0.0404(18) -0.0028(13) -0.0054(12) 0.0023(11)
F214 0.0271(15) 0.0131(14) 0.0275(16) 0.0006(12) -0.0001(12) -0.0006(11)
F215 0.0340(17) 0.0417(18) 0.0256(17) 0.0125(14) -0.0002(13) 0.0040(14)
F216 0.0383(18) 0.054(2) 0.0224(18) -0.0080(14) -0.0034(14) -0.0016(15)
F217 0.0403(18) 0.0386(19) 0.042(2) -0.0253(15) 0.0016(15) -0.0109(14)
F218 0.0303(16) 0.0131(14) 0.0407(19) -0.0063(12) 0.0015(13) -0.0046(12)
F220 0.0164(14) 0.0273(16) 0.058(2) 0.0078(14) 0.0016(14) -0.0008(12)
```

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F221 0.0280(18) 0.040(2) 0.103(3) 0.019(2) 0.0141(18) -0.0090(15)
F222 0.067(2) 0.0327(19) 0.066(3) 0.0135(17) 0.035(2) -0.0074(17)
F223 0.083(3) 0.0275(17) 0.032(2) 0.0062(14) -0.0026(18) -0.0120(17)
F224 0.0407(18) 0.0266(16) 0.0306(18) 0.0072(13) -0.0070(14) -0.0092(13)
C21 0.019(2) 0.014(2) 0.014(2) -0.0037(18) -0.0014(18) 0.0018(17)
C22 0.020(2) 0.014(2) 0.022(3) 0.000(2) -0.001(2) -0.0020(18)
C23 0.021(2) 0.020(2) 0.028(3) -0.003(2) 0.003(2) 0.0107(19)
C24 0.014(2) 0.024(2) 0.031(3) -0.003(2) 0.000(2) 0.0017(19)
C25 0.019(2) 0.018(2) 0.028(3) -0.003(2) -0.001(2) -0.0047(19)
C26 0.014(2) 0.012(2) 0.024(3) -0.0032(19) 0.0005(19) 0.0035(17)
C27 0.019(2) 0.011(2) 0.030(3) 0.001(2) 0.006(2) -0.0031(18)
C28 0.024(2) 0.012(2) 0.027(3) 0.003(2) 0.006(2) 0.0030(19)
C29 0.035(3) 0.017(2) 0.022(3) 0.004(2) 0.014(2) -0.005(2)
C210 0.025(3) 0.016(2) 0.048(3) -0.001(2) 0.021(2) 0.005(2)
C211 0.015(2) 0.017(2) 0.045(3) 0.005(2) 0.008(2) 0.0015(19)
C212 0.015(2) 0.016(2) 0.028(3) 0.003(2) 0.006(2) -0.0041(18)
C213 0.011(2) 0.014(2) 0.030(3) -0.0065(19) -0.0016(19) -0.0011(17)
C214 0.012(2) 0.020(2) 0.026(3) -0.005(2) -0.001(2) 0.0035(18)
C215 0.011(2) 0.028(3) 0.030(3) 0.002(2) -0.002(2) 0.0038(19)
C216 0.016(2) 0.036(3) 0.023(3) -0.009(2) -0.003(2) 0.007(2)
C217 0.016(2) 0.029(3) 0.034(3) -0.014(2) -0.004(2) 0.000(2)
C218 0.015(2) 0.019(2) 0.028(3) -0.004(2) 0.003(2) -0.0016(19)
C219 0.024(2) 0.011(2) 0.028(3) -0.005(2) 0.010(2) 0.0035(18)
C220 0.023(2) 0.013(2) 0.043(3) 0.001(2) 0.010(2) 0.0052(19)
C221 0.022(3) 0.024(3) 0.060(4) 0.000(3) 0.017(2) -0.001(2)
C222 0.042(3) 0.017(3) 0.042(3) 0.004(2) 0.025(2) -0.002(2)
C223 0.053(3) 0.014(2) 0.025(3) -0.005(2) 0.013(2) 0.000(2)
C224 0.034(3) 0.018(2) 0.025(3) -0.004(2) 0.008(2) 0.000(2)
B2 0.016(2) 0.014(2) 0.024(3) -0.001(2) 0.001(2) -0.0014(19)
Ti1 0.0195(5) 0.0224(5) 0.0310(6) 0.0053(4) 0.0005(4) 0.0030(4)
C11 0.035(3) 0.020(2) 0.030(3) 0.001(2) -0.010(2) 0.005(2)
C12 0.036(3) 0.058(4) 0.063(4) -0.014(3) -0.018(3) 0.015(3)
C13 0.051(4) 0.094(5) 0.080(5) 0.001(5) -0.005(4) -0.002(4)
C14 0.045(3) 0.064(4) 0.065(4) 0.014(3) -0.013(3) -0.025(3)
C15 0.044(3) 0.022(3) 0.049(3) 0.001(2) -0.016(3) 0.000(2)
C16 0.037(3) 0.014(2) 0.022(2) -0.005(2) -0.003(2) 0.0075(19)
C17 0.029(2) 0.017(2) 0.036(3) 0.002(2) 0.005(2) 0.002(2)
C18 0.046(4) 0.027(3) 0.063(4) 0.000(3) 0.016(3) 0.012(3)
C19 0.041(3) 0.027(3) 0.041(4) 0.001(3) 0.016(3) 0.009(2)
C110 0.018(2) 0.025(2) 0.032(3) 0.009(2) -0.003(2) -0.0019(19)
C111 0.027(3) 0.031(3) 0.039(3) 0.001(2) -0.009(2) -0.003(2)
C112 0.034(3) 0.107(4) 0.049(4) -0.042(3) -0.011(3) 0.012(3)
C113 0.020(3) 0.159(6) 0.040(3) 0.062(4) -0.003(2) -0.010(3)
C114 0.018(2) 0.041(3) 0.065(4) 0.026(3) -0.009(2) 0.000(2)
C115 0.033(3) 0.037(3) 0.040(3) -0.002(3) -0.001(3) 0.006(2)
C116 0.034(3) 0.039(3) 0.051(4) 0.015(3) 0.005(3) 0.000(2)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
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_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Ti1     C112       2.488(7)                    .      .                    yes
 Ti1     C113       2.475(6)                    .      .                    yes
 Ti1     C11        2.463(5)                    .      .                    yes
 Ti1     C15        2.465(6)                    .      .                    yes
 Ti1     C16        2.425(5)                    .      .                    yes
 Ti1     C110       2.399(4)                    .      .                    yes
 Ti1     C111       2.430(5)                    .      .                    yes
 Ti1     C115       2.131(5)                    .      .                    yes
 Ti1     C116       2.119(6)                    .      .                    yes
 Ti1     C114       2.405(5)                    .      .                    yes
 F22     C22        1.355(5)                    .      .                    yes
 F23     C23        1.355(5)                    .      .                    yes
 F24     C24        1.352(5)                    .      .                    yes
 F25     C25        1.351(5)                    .      .                    yes
 F26     C26        1.368(5)                    .      .                    yes
 F28     C28        1.343(5)                    .      .                    yes
 F29     C29        1.345(6)                    .      .                    yes
 F210    C210       1.350(5)                    .      .                    yes
 F211    C211       1.356(5)                    .      .                    yes
 F212    C212       1.364(5)                    .      .                    yes
 F214    C214       1.357(5)                    .      .                    yes
 F215    C215       1.341(6)                    .      .                    yes
 F216    C216       1.338(6)                    .      .                    yes
 F217    C217       1.345(6)                    .      .                    yes
 F218    C218       1.352(5)                    .      .                    yes
 F220    C220       1.359(6)                    .      .                    yes
 F221    C221       1.351(6)                    .      .                    yes
 F222    C222       1.349(6)                    .      .                    yes
 F223    C223       1.349(6)                    .      .                    yes
 F224    C224       1.345(6)                    .      .                    yes
 C21     C22        1.398(6)                    .      .                    no
 C21     B2         1.644(7)                    .      .                    yes
 C21     C26        1.393(6)                    .      .                    no
 C22     C23        1.378(6)                    .      .                    no
 C23     C24        1.375(6)                    .      .                    no
 C24     C25        1.374(6)                    .      .                    no
 C25     C26        1.380(6)                    .      .                    no
 C27     C28        1.399(7)                    .      .                    no
 C27     B2         1.668(7)                    .      .                    yes
 C27     C212       1.394(6)                    .      .                    no
 C28     C29        1.378(6)                    .      .                    no
 C29     C210       1.379(7)                    .      .                    no
 C210    C211       1.365(8)                    .      .                    no
 C11     C12        1.358(8)                    .      .                    no
 C11     C16        1.405(7)                    .      .                    no
 C211    C212       1.377(6)                    .      .                    no
 C12     C13       1.229(11)                    .      .                    no
 C13     C14       1.250(11)                    .      .                    no
 C213    C218       1.384(6)                    .      .                    no
 C213    C214       1.398(6)                    .      .                    no
 C213    B2         1.649(7)                    .      .                    yes
 C14     C15        1.319(8)                    .      .                    no
 C214    C215       1.393(7)                    .      .                    no
 C215    C216       1.374(7)                    .      .                    no
 C15     C16        1.421(7)                    .      .                    no
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 C216    C217       1.378(7)                    .      .                 no
 C16     C17        1.539(8)                    .      .                 no
 C217    C218       1.403(7)                    .      .                 no
 C17     C18        1.532(7)                    .      .                 no
 C17     C19        1.531(7)                    .      .                 no
 C17     C110       1.545(7)                    .      .                 no
 C219    C224       1.383(7)                    .      .                 no
 C219    B2         1.658(7)                    .      .                 yes
 C219    C220       1.388(6)                    .      .                 no
 C220    C221       1.390(7)                    .      .                 no
 C221    C222       1.380(8)                    .      .                 no
 C222    C223       1.357(8)                    .      .                 no
 C223    C224       1.396(7)                    .      .                 no
 C110    C111       1.407(8)                    .      .                 no
 C110    C114       1.410(8)                    .      .                 no
 C111    C112      1.386(10)                    .      .                 no
 C11     H11          0.9500                    .      .                 no
 C112    C113      1.554(12)                    .      .                 no
 C12     H12          0.9500                    .      .                 no
 C113    C114       1.519(9)                    .      .                 no
 C13     H13          0.9500                    .      .                 no
 C14     H14          0.9500                    .      .                 no
 C15     H15          0.9500                    .      .                 no
 C18     H18          0.9800                    .      .                 no
 C18     H18'         0.9800                    .      .                 no
 C18     H18"         0.9800                    .      .                 no
 C19     H19          0.9800                    .      .                 no
 C19     H19'         0.9800                    .      .                 no
 C19     H19"         0.9800                    .      .                 no
 C111    H111         0.9500                    .      .                 no
 C112    H112         0.9500                    .      .                 no
 C113    H113         0.9500                    .      .                 no
 C114    H114         0.9500                    .      .                 no
 C115    H115'        0.9800                    .      .                 no
 C115    H115"        0.9800                    .      .                 no
 C115    H115         0.9800                    .      .                 no
 C116    H116'        0.9800                    .      .                 no
 C116    H116"        0.9800                    .      .                 no
 C116    H116         0.9800                    .      .                 no

loop_
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_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 C15     Ti1     C116        90.6(2)             .      .      .          yes
 C16     Ti1     C110      57.22(18)             .      .      .          yes
 C16     Ti1     C111      77.69(18)             .      .      .          yes
 C16     Ti1     C112       109.6(2)             .      .      .          yes
 C16     Ti1     C113     112.96(19)             .      .      .          yes
 C16     Ti1     C114      78.64(18)             .      .      .          yes
 C16     Ti1     C115     127.97(19)             .      .      .          yes
 C16     Ti1     C116     124.00(18)             .      .      .          yes
 C110    Ti1     C111      33.87(18)             .      .      .          yes
 C110    Ti1     C112        56.4(2)             .      .      .          yes
 C110    Ti1     C113      58.08(18)             .      .      .          yes
 C110    Ti1     C114      34.13(18)             .      .      .          yes
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C110	Ti1	C115	128.3(2)	.	.	.	yes
C110	Ti1	C116	124.5(2)	.	.	.	yes
C111	Ti1	C112	32.7(2)	.	.	.	yes
C11	Ti1	C15	57.13(18)	.	.	.	yes
C11	Ti1	C16	33.39(16)	.	.	.	yes
C11	Ti1	C110	76.65(18)	.	.	.	yes
C11	Ti1	C111	79.23(18)	.	.	.	yes
C11	Ti1	C112	109.8(2)	.	.	.	yes
C11	Ti1	C113	133.48(19)	.	.	.	yes
C11	Ti1	C114	106.90(19)	.	.	.	yes
C11	Ti1	C115	94.6(2)	.	.	.	yes
C11	Ti1	C116	139.0(2)	.	.	.	yes
C15	Ti1	C16	33.76(16)	.	.	.	yes
C15	Ti1	C110	78.22(18)	.	.	.	yes
C15	Ti1	C111	107.39(18)	.	.	.	yes
C15	Ti1	C112	134.5(2)	.	.	.	yes
C15	Ti1	C113	117.0(2)	.	.	.	yes
C15	Ti1	C114	82.12(18)	.	.	.	yes
C15	Ti1	C115	138.4(2)	.	.	.	yes
C111	Ti1	C113	57.7(2)	.	.	.	yes
C111	Ti1	C114	57.11(18)	.	.	.	yes
C111	Ti1	C115	94.53(19)	.	.	.	yes
C111	Ti1	C116	139.1(2)	.	.	.	yes
C112	Ti1	C113	36.5(3)	.	.	.	yes
C112	Ti1	C114	59.0(2)	.	.	.	yes
C112	Ti1	C115	80.8(2)	.	.	.	yes
C112	Ti1	C116	111.0(2)	.	.	.	yes
C113	Ti1	C114	36.2(2)	.	.	.	yes
C113	Ti1	C115	104.6(2)	.	.	.	yes
C113	Ti1	C116	81.4(2)	.	.	.	yes
C114	Ti1	C115	138.7(2)	.	.	.	yes
C114	Ti1	C116	90.9(2)	.	.	.	yes
C115	Ti1	C116	95.4(2)	.	.	.	yes
C26	C21	B2	127.4(4)	.	.	.	yes
C22	C21	C26	112.4(4)	.	.	.	no
C22	C21	B2	119.8(4)	.	.	.	yes
C21	C22	C23	124.8(4)	.	.	.	no
F22	C22	C21	118.7(4)	.	.	.	yes
F22	C22	C23	116.5(4)	.	.	.	yes
F23	C23	C22	120.1(4)	.	.	.	yes
F23	C23	C24	120.5(4)	.	.	.	yes
C22	C23	C24	119.4(4)	.	.	.	no
F24	C24	C23	120.8(4)	.	.	.	yes
F24	C24	C25	120.1(4)	.	.	.	yes
C23	C24	C25	119.1(4)	.	.	.	no
C24	C25	C26	119.4(4)	.	.	.	no
F25	C25	C24	119.9(4)	.	.	.	yes
F25	C25	C26	120.7(4)	.	.	.	yes
F26	C26	C21	121.2(4)	.	.	.	yes
F26	C26	C25	114.0(3)	.	.	.	yes
C21	C26	C25	124.9(4)	.	.	.	no
C28	C27	B2	120.2(4)	.	.	.	yes
C212	C27	B2	126.3(4)	.	.	.	yes
C28	C27	C212	113.0(4)	.	.	.	no
F28	C28	C27	119.3(4)	.	.	.	yes
F28	C28	C29	116.9(4)	.	.	.	yes
C27	C28	C29	123.9(4)	.	.	.	no
F29	C29	C28	120.6(4)	.	.	.	yes
C28	C29	C210	119.7(5)	.	.	.	no
F29	C29	C210	119.7(4)	.	.	.	yes
C29	C210	C211	119.2(4)	.	.	.	no

F210	C210	C29	121.1(5)	.	.	.	yes
F210	C210	C211	119.7(4)	.	.	.	yes
C12	C11	C16	118.8(5)	.	.	.	no
Ti1	C11	C12	80.2(3)	.	.	.	yes
Ti1	C11	C16	71.8(3)	.	.	.	yes
F211	C211	C212	120.1(4)	.	.	.	yes
C210	C211	C212	119.5(4)	.	.	.	no
F211	C211	C210	120.4(4)	.	.	.	yes
F212	C212	C211	115.0(4)	.	.	.	yes
C27	C212	C211	124.7(4)	.	.	.	no
F212	C212	C27	120.3(4)	.	.	.	yes
C11	C12	C13	122.8(7)	.	.	.	no
C218	C213	B2	127.3(4)	.	.	.	yes
C214	C213	C218	113.6(4)	.	.	.	no
C214	C213	B2	119.1(4)	.	.	.	yes
C12	C13	C14	122.1(8)	.	.	.	no
C13	C14	C15	122.5(7)	.	.	.	no
F214	C214	C213	119.6(4)	.	.	.	yes
F214	C214	C215	115.7(4)	.	.	.	yes
C213	C214	C215	124.7(4)	.	.	.	no
F215	C215	C216	120.4(4)	.	.	.	yes
C214	C215	C216	118.9(5)	.	.	.	no
C14	C15	C16	120.1(5)	.	.	.	no
F215	C215	C214	120.7(4)	.	.	.	yes
Ti1	C15	C14	80.5(4)	.	.	.	yes
Ti1	C15	C16	71.6(3)	.	.	.	yes
F216	C216	C215	120.5(5)	.	.	.	yes
Ti1	C16	C11	74.8(3)	.	.	.	yes
Ti1	C16	C15	74.7(3)	.	.	.	yes
Ti1	C16	C17	102.4(3)	.	.	.	yes
C11	C16	C15	113.1(5)	.	.	.	no
C11	C16	C17	121.5(4)	.	.	.	no
C15	C16	C17	122.5(4)	.	.	.	no
F216	C216	C217	120.2(5)	.	.	.	yes
C215	C216	C217	119.3(5)	.	.	.	no
C16	C17	C110	97.0(4)	.	.	.	no
C16	C17	C18	113.3(4)	.	.	.	no
C16	C17	C19	112.8(4)	.	.	.	no
F217	C217	C216	120.8(5)	.	.	.	yes
F217	C217	C218	119.5(4)	.	.	.	yes
C216	C217	C218	119.8(5)	.	.	.	no
C19	C17	C110	113.3(4)	.	.	.	no
C18	C17	C19	107.7(4)	.	.	.	no
C18	C17	C110	112.7(4)	.	.	.	no
F218	C218	C217	114.8(4)	.	.	.	yes
F218	C218	C213	121.6(4)	.	.	.	yes
C213	C218	C217	123.6(4)	.	.	.	no
C220	C219	C224	113.8(4)	.	.	.	no
C220	C219	B2	119.8(4)	.	.	.	yes
C224	C219	B2	125.9(4)	.	.	.	yes
C219	C220	C221	124.5(5)	.	.	.	no
F220	C220	C219	120.1(4)	.	.	.	yes
F220	C220	C221	115.5(4)	.	.	.	yes
F221	C221	C220	120.9(5)	.	.	.	yes
F221	C221	C222	120.6(5)	.	.	.	yes
C220	C221	C222	118.5(5)	.	.	.	no
C221	C222	C223	119.7(5)	.	.	.	no
F222	C222	C221	119.5(5)	.	.	.	yes
F222	C222	C223	120.8(5)	.	.	.	yes
F223	C223	C224	119.6(5)	.	.	.	yes
F223	C223	C222	120.6(4)	.	.	.	yes

C222	C223	C224	119.8(5)	.	.	.	no
F224	C224	C219	120.9(4)	.	.	.	yes
F224	C224	C223	115.5(4)	.	.	.	yes
C219	C224	C223	123.5(5)	.	.	.	no
Ti1	C110	C17	103.3(3)	.	.	.	yes
Ti1	C110	C114	73.2(3)	.	.	.	yes
C17	C110	C111	123.4(5)	.	.	.	no
Ti1	C110	C111	74.2(3)	.	.	.	yes
C111	C110	C114	110.3(5)	.	.	.	no
C17	C110	C114	123.2(5)	.	.	.	no
Ti1	C111	C112	76.0(4)	.	.	.	yes
C110	C111	C112	111.7(5)	.	.	.	no
Ti1	C111	C110	71.9(3)	.	.	.	yes
C16	C11	H11	121.00	.	.	.	no
Ti1	C11	H11	118.00	.	.	.	no
C12	C11	H11	121.00	.	.	.	no
Ti1	C112	C111	71.3(4)	.	.	.	yes
C11	C12	H12	119.00	.	.	.	no
Ti1	C112	C113	71.3(3)	.	.	.	yes
C111	C112	C113	107.0(6)	.	.	.	no
C13	C12	H12	119.00	.	.	.	no
C14	C13	H13	119.00	.	.	.	no
C112	C113	C114	103.2(5)	.	.	.	no
Ti1	C113	C112	72.2(4)	.	.	.	yes
C12	C13	H13	119.00	.	.	.	no
Ti1	C113	C114	69.4(3)	.	.	.	yes
C13	C14	H14	119.00	.	.	.	no
C15	C14	H14	119.00	.	.	.	no
Ti1	C114	C110	72.7(3)	.	.	.	yes
Ti1	C114	C113	74.4(3)	.	.	.	yes
C110	C114	C113	107.8(5)	.	.	.	no
Ti1	C15	H15	119.00	.	.	.	no
C16	C15	H15	120.00	.	.	.	no
C14	C15	H15	120.00	.	.	.	no
C17	C18	H18	109.00	.	.	.	no
C17	C18	H18'	109.00	.	.	.	no
H18	C18	H18'	110.00	.	.	.	no
H18	C18	H18"	109.00	.	.	.	no
C17	C18	H18"	109.00	.	.	.	no
H18'	C18	H18"	109.00	.	.	.	no
C17	C19	H19"	109.00	.	.	.	no
H19	C19	H19'	109.00	.	.	.	no
C17	C19	H19'	109.00	.	.	.	no
H19'	C19	H19"	109.00	.	.	.	no
H19	C19	H19"	109.00	.	.	.	no
C17	C19	H19	109.00	.	.	.	no
Ti1	C111	H111	120.00	.	.	.	no
C112	C111	H111	124.00	.	.	.	no
C110	C111	H111	124.00	.	.	.	no
Ti1	C112	H112	123.00	.	.	.	no
C111	C112	H112	127.00	.	.	.	no
C113	C112	H112	126.00	.	.	.	no
Ti1	C113	H113	122.00	.	.	.	no
C112	C113	H113	128.00	.	.	.	no
C114	C113	H113	128.00	.	.	.	no
C110	C114	H114	126.00	.	.	.	no
C113	C114	H114	126.00	.	.	.	no
Ti1	C114	H114	119.00	.	.	.	no
H115'	C115	H115"	110.00	.	.	.	no
Ti1	C115	H115	109.00	.	.	.	no
H115'	C115	H115	109.00	.	.	.	no

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 H115"   C115    H115         110.00            .       .       .          no
 Ti1     C115    H115"        109.00            .       .       .          no
 Ti1     C115    H115'        109.00            .       .       .          no
 Ti1     C116    H116'        110.00            .       .       .          no
 Ti1     C116    H116         109.00            .       .       .          no
 H116'   C116    H116"        109.00            .       .       .          no
 H116'   C116    H116         109.00            .       .       .          no
 H116"   C116    H116         109.00            .       .       .          no
 Ti1     C116    H116"        110.00            .       .       .          no
 C27     B2      C219       100.3(4)            .       .       .          yes
 C213    B2      C219       114.7(4)            .       .       .          yes
 C21     B2      C27        114.8(4)            .       .       .          yes
 C21     B2      C213       102.0(4)            .       .       .          yes
 C21     B2      C219       113.2(4)            .       .       .          yes
 C27     B2      C213       112.4(4)            .       .       .          yes

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 C15     Ti1     C114    C113      -164.6(4)     .       .       .       .   no
 C16     Ti1     C114    C110        46.5(3)     .       .       .       .   no
 C16     Ti1     C114    C113       161.3(4)     .       .       .       .   no
 C110    Ti1     C114    C113       114.8(5)     .       .       .       .   no
 C111    Ti1     C114    C110       -36.1(3)     .       .       .       .   no
 C111    Ti1     C114    C113        78.7(4)     .       .       .       .   no
 C112    Ti1     C114    C110       -74.8(4)     .       .       .       .   no
 C112    Ti1     C114    C113        40.0(4)     .       .       .       .   no
 C113    Ti1     C114    C110      -114.8(5)     .       .       .       .   no
 C115    Ti1     C114    C110       -89.7(4)     .       .       .       .   no
 C115    Ti1     C114    C113        25.1(5)     .       .       .       .   no
 C116    Ti1     C114    C110       171.1(3)     .       .       .       .   no
 C116    Ti1     C114    C113       -74.1(4)     .       .       .       .   no
 C110    Ti1     C15     C14       -173.2(4)     .       .       .       .   no
 C110    Ti1     C15     C16        -46.9(3)     .       .       .       .   no
 C111    Ti1     C15     C14       -155.8(4)     .       .       .       .   no
 C111    Ti1     C15     C16        -29.5(3)     .       .       .       .   no
 C112    Ti1     C15     C14       -177.6(4)     .       .       .       .   no
 C112    Ti1     C15     C16        -51.3(4)     .       .       .       .   no
 C113    Ti1     C15     C14        142.2(4)     .       .       .       .   no
 C113    Ti1     C15     C16        -91.5(4)     .       .       .       .   no
 C114    Ti1     C15     C14        152.4(4)     .       .       .       .   no
 C114    Ti1     C15     C16        -81.3(3)     .       .       .       .   no
 C115    Ti1     C15     C14        -37.3(5)     .       .       .       .   no
 C115    Ti1     C15     C16         89.0(4)     .       .       .       .   no
 C116    Ti1     C15     C14         61.6(4)     .       .       .       .   no
 C116    Ti1     C15     C16       -172.1(3)     .       .       .       .   no
 C11     Ti1     C16     C15       -119.7(5)     .       .       .       .   no
 C11     Ti1     C16     C17        119.7(4)     .       .       .       .   no
 C15     Ti1     C16     C11        119.7(5)     .       .       .       .   no
 C15     Ti1     C16     C17       -120.7(4)     .       .       .       .   no
 C110    Ti1     C16     C11       -118.6(3)     .       .       .       .   no
 C110    Ti1     C16     C15        121.8(3)     .       .       .       .   no
 C110    Ti1     C16     C17          1.1(2)     .       .       .       .   no
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C111	Ti1	C16	C11	-89.1(3)	.	.	.	.	no
C111	Ti1	C16	C15	151.3(3)	.	.	.	.	no
C111	Ti1	C16	C17	30.6(3)	.	.	.	.	no
C112	Ti1	C16	C11	-96.6(4)	.	.	.	.	no
C112	Ti1	C16	C15	143.8(3)	.	.	.	.	no
C112	Ti1	C16	C17	23.1(3)	.	.	.	.	no
C113	Ti1	C16	C11	-135.7(4)	.	.	.	.	no
C113	Ti1	C16	C15	104.7(4)	.	.	.	.	no
C113	Ti1	C16	C17	-16.0(4)	.	.	.	.	no
C114	Ti1	C16	C11	-147.5(3)	.	.	.	.	no
C114	Ti1	C16	C15	92.8(3)	.	.	.	.	no
C114	Ti1	C16	C17	-27.9(3)	.	.	.	.	no
C115	Ti1	C16	C11	-3.0(4)	.	.	.	.	no
C115	Ti1	C16	C15	-122.6(3)	.	.	.	.	no
C115	Ti1	C16	C17	116.7(3)	.	.	.	.	no
C116	Ti1	C16	C11	129.2(3)	.	.	.	.	no
C116	Ti1	C16	C15	9.5(4)	.	.	.	.	no
C116	Ti1	C16	C17	-111.2(3)	.	.	.	.	no
C11	Ti1	C110	C17	-30.9(3)	.	.	.	.	no
C11	Ti1	C110	C111	90.5(3)	.	.	.	.	no
C11	Ti1	C110	C114	-152.0(3)	.	.	.	.	no
C15	Ti1	C110	C17	27.8(3)	.	.	.	.	no
C15	Ti1	C110	C111	149.2(3)	.	.	.	.	no
C15	Ti1	C110	C114	-93.3(3)	.	.	.	.	no
C16	Ti1	C110	C17	-1.1(2)	.	.	.	.	no
C16	Ti1	C110	C111	120.3(4)	.	.	.	.	no
C16	Ti1	C110	C114	-122.2(4)	.	.	.	.	no
C111	Ti1	C110	C17	-121.4(5)	.	.	.	.	no
C111	Ti1	C110	C114	117.5(5)	.	.	.	.	no
C112	Ti1	C110	C17	-156.0(4)	.	.	.	.	no
C112	Ti1	C110	C111	-34.6(3)	.	.	.	.	no
C112	Ti1	C110	C114	82.9(4)	.	.	.	.	no
C113	Ti1	C110	C17	160.3(4)	.	.	.	.	no
C113	Ti1	C110	C111	-78.3(4)	.	.	.	.	no
C113	Ti1	C110	C114	39.2(4)	.	.	.	.	no
C114	Ti1	C110	C17	121.1(5)	.	.	.	.	no
C114	Ti1	C110	C111	-117.5(5)	.	.	.	.	no
C115	Ti1	C110	C17	-116.2(3)	.	.	.	.	no
C115	Ti1	C110	C111	5.2(4)	.	.	.	.	no
C115	Ti1	C110	C114	122.7(3)	.	.	.	.	no
C116	Ti1	C110	C17	110.3(3)	.	.	.	.	no
C116	Ti1	C110	C111	-128.3(3)	.	.	.	.	no
C116	Ti1	C110	C114	-10.8(4)	.	.	.	.	no
C11	Ti1	C111	C110	-82.1(3)	.	.	.	.	no
C11	Ti1	C111	C112	159.1(4)	.	.	.	.	no
C15	Ti1	C111	C110	-31.7(3)	.	.	.	.	no
C15	Ti1	C111	C112	-150.6(4)	.	.	.	.	no
C16	Ti1	C111	C110	-48.0(3)	.	.	.	.	no
C16	Ti1	C111	C112	-166.9(4)	.	.	.	.	no
C110	Ti1	C111	C112	-118.9(5)	.	.	.	.	no
C112	Ti1	C111	C110	118.9(5)	.	.	.	.	no
C113	Ti1	C111	C110	79.7(4)	.	.	.	.	no
C113	Ti1	C111	C112	-39.2(4)	.	.	.	.	no
C114	Ti1	C111	C110	36.3(3)	.	.	.	.	no
C114	Ti1	C111	C112	-82.5(4)	.	.	.	.	no
C115	Ti1	C111	C110	-175.9(3)	.	.	.	.	no
C115	Ti1	C111	C112	65.2(4)	.	.	.	.	no
C116	Ti1	C111	C110	80.5(4)	.	.	.	.	no
C116	Ti1	C111	C112	-38.4(5)	.	.	.	.	no
C11	Ti1	C112	C111	-21.9(4)	.	.	.	.	no
C11	Ti1	C112	C113	-138.0(3)	.	.	.	.	no

C15	Ti1	C112	C111	41.1(5)	.	.	.	no
C15	Ti1	C112	C113	-75.0(5)	.	.	.	no
C16	Ti1	C112	C111	13.6(4)	.	.	.	no
C16	Ti1	C112	C113	-102.4(3)	.	.	.	no
C110	Ti1	C112	C111	35.9(3)	.	.	.	no
C110	Ti1	C112	C113	-80.2(4)	.	.	.	no
C111	Ti1	C112	C113	-116.1(5)	.	.	.	no
C113	Ti1	C112	C111	116.1(5)	.	.	.	no
C114	Ti1	C112	C111	76.4(4)	.	.	.	no
C114	Ti1	C112	C113	-39.7(3)	.	.	.	no
C115	Ti1	C112	C111	-113.5(4)	.	.	.	no
C115	Ti1	C112	C113	130.4(4)	.	.	.	no
C116	Ti1	C112	C111	154.2(4)	.	.	.	no
C116	Ti1	C112	C113	38.1(4)	.	.	.	no
C11	Ti1	C113	C112	60.2(5)	.	.	.	no
C11	Ti1	C113	C114	-52.0(5)	.	.	.	no
C15	Ti1	C113	C112	129.4(4)	.	.	.	no
C15	Ti1	C113	C114	17.2(4)	.	.	.	no
C16	Ti1	C113	C112	92.2(4)	.	.	.	no
C16	Ti1	C113	C114	-20.0(4)	.	.	.	no
C110	Ti1	C113	C112	75.3(4)	.	.	.	no
C110	Ti1	C113	C114	-36.9(3)	.	.	.	no
C111	Ti1	C113	C112	35.1(4)	.	.	.	no
C111	Ti1	C113	C114	-77.1(3)	.	.	.	no
C112	Ti1	C113	C114	-112.2(5)	.	.	.	no
C15	Ti1	C11	C12	89.8(4)	.	.	.	no
C15	Ti1	C11	C16	-35.1(3)	.	.	.	no
C16	Ti1	C11	C12	124.9(5)	.	.	.	no
C110	Ti1	C11	C12	174.3(4)	.	.	.	no
C110	Ti1	C11	C16	49.4(3)	.	.	.	no
C111	Ti1	C11	C12	-151.2(4)	.	.	.	no
C111	Ti1	C11	C16	83.9(3)	.	.	.	no
C112	Ti1	C11	C12	-139.3(4)	.	.	.	no
C112	Ti1	C11	C16	95.8(3)	.	.	.	no
C113	Ti1	C11	C12	-172.6(4)	.	.	.	no
C113	Ti1	C11	C16	62.5(4)	.	.	.	no
C114	Ti1	C11	C12	158.3(4)	.	.	.	no
C114	Ti1	C11	C16	33.4(3)	.	.	.	no
C115	Ti1	C11	C12	-57.4(4)	.	.	.	no
C115	Ti1	C11	C16	177.7(3)	.	.	.	no
C116	Ti1	C11	C12	46.3(5)	.	.	.	no
C116	Ti1	C11	C16	-78.6(4)	.	.	.	no
C11	Ti1	C15	C14	-91.6(4)	.	.	.	no
C11	Ti1	C15	C16	34.7(3)	.	.	.	no
C16	Ti1	C15	C14	-126.3(5)	.	.	.	no
C115	Ti1	C113	C114	-163.2(3)	.	.	.	no
C116	Ti1	C113	C112	-144.4(4)	.	.	.	no
C116	Ti1	C113	C114	103.4(4)	.	.	.	no
C11	Ti1	C114	C110	28.5(3)	.	.	.	no
C11	Ti1	C114	C113	143.3(4)	.	.	.	no
C15	Ti1	C114	C110	80.6(3)	.	.	.	no
C114	Ti1	C113	C112	112.2(5)	.	.	.	no
C115	Ti1	C113	C112	-51.0(4)	.	.	.	no
B2	C21	C22	F22	5.2(6)	.	.	.	no
B2	C21	C22	C23	-175.2(4)	.	.	.	no
C22	C21	C26	F26	-177.7(4)	.	.	.	no
C22	C21	C26	C25	1.7(7)	.	.	.	no
B2	C21	C26	F26	-5.6(7)	.	.	.	no
C26	C21	C22	F22	178.0(4)	.	.	.	no
C26	C21	C22	C23	-2.4(7)	.	.	.	no
C26	C21	B2	C219	132.7(5)	.	.	.	no

C26	C21	B2	C213	-103.5(5)	.	.	.	.	no
C26	C21	B2	C27	18.3(7)	.	.	.	.	no
B2	C21	C26	C25	173.9(5)	.	.	.	.	no
C22	C21	B2	C27	-170.1(4)	.	.	.	.	no
C22	C21	B2	C213	68.1(5)	.	.	.	.	no
C22	C21	B2	C219	-55.7(6)	.	.	.	.	no
C21	C22	C23	C24	1.1(7)	.	.	.	.	no
F22	C22	C23	F23	-0.3(6)	.	.	.	.	no
C21	C22	C23	F23	-179.8(4)	.	.	.	.	no
F22	C22	C23	C24	-179.4(4)	.	.	.	.	no
F23	C23	C24	F24	0.4(7)	.	.	.	.	no
C22	C23	C24	C25	1.2(7)	.	.	.	.	no
F23	C23	C24	C25	-177.9(4)	.	.	.	.	no
C22	C23	C24	F24	179.5(4)	.	.	.	.	no
C23	C24	C25	C26	-1.8(7)	.	.	.	.	no
F24	C24	C25	F25	0.7(7)	.	.	.	.	no
F24	C24	C25	C26	179.9(4)	.	.	.	.	no
C23	C24	C25	F25	179.0(4)	.	.	.	.	no
F25	C25	C26	F26	-1.1(6)	.	.	.	.	no
F25	C25	C26	C21	179.5(4)	.	.	.	.	no
C24	C25	C26	F26	179.8(4)	.	.	.	.	no
C24	C25	C26	C21	0.3(7)	.	.	.	.	no
B2	C27	C28	F28	-4.5(6)	.	.	.	.	no
B2	C27	C28	C29	175.1(4)	.	.	.	.	no
C212	C27	C28	C29	2.7(6)	.	.	.	.	no
C212	C27	B2	C213	-21.4(6)	.	.	.	.	no
C212	C27	B2	C219	100.9(5)	.	.	.	.	no
C28	C27	C212	F212	178.3(4)	.	.	.	.	no
C28	C27	B2	C21	51.3(6)	.	.	.	.	no
C28	C27	B2	C213	167.3(4)	.	.	.	.	no
C28	C27	B2	C219	-70.4(5)	.	.	.	.	no
C212	C27	B2	C21	-137.4(5)	.	.	.	.	no
C212	C27	C28	F28	-176.9(4)	.	.	.	.	no
B2	C27	C212	C211	-174.1(4)	.	.	.	.	no
B2	C27	C212	F212	6.5(7)	.	.	.	.	no
C28	C27	C212	C211	-2.2(6)	.	.	.	.	no
C27	C28	C29	F29	176.8(4)	.	.	.	.	no
C27	C28	C29	C210	-1.7(7)	.	.	.	.	no
F28	C28	C29	F29	-3.6(6)	.	.	.	.	no
F28	C28	C29	C210	177.9(4)	.	.	.	.	no
F29	C29	C210	C211	-178.6(4)	.	.	.	.	no
C28	C29	C210	F210	179.9(4)	.	.	.	.	no
C28	C29	C210	C211	-0.2(7)	.	.	.	.	no
F29	C29	C210	F210	1.4(7)	.	.	.	.	no
F210	C210	C211	C212	-179.4(4)	.	.	.	.	no
F210	C210	C211	F211	-0.4(6)	.	.	.	.	no
C29	C210	C211	F211	179.7(4)	.	.	.	.	no
C29	C210	C211	C212	0.6(7)	.	.	.	.	no
F211	C211	C212	F212	1.1(6)	.	.	.	.	no
Ti1	C11	C12	C13	-65.9(7)	.	.	.	.	no
C16	C11	C12	C13	-3.1(9)	.	.	.	.	no
Ti1	C11	C16	C15	65.6(4)	.	.	.	.	no
Ti1	C11	C16	C17	-95.4(4)	.	.	.	.	no
F211	C211	C212	C27	-178.4(4)	.	.	.	.	no
C210	C211	C212	F212	-179.8(4)	.	.	.	.	no
C210	C211	C212	C27	0.7(7)	.	.	.	.	no
C12	C11	C16	C17	-162.7(5)	.	.	.	.	no
C12	C11	C16	Ti1	-67.3(5)	.	.	.	.	no
C12	C11	C16	C15	-1.7(7)	.	.	.	.	no
C11	C12	C13	C14	9.0(13)	.	.	.	.	no
C12	C13	C14	C15	-9.6(14)	.	.	.	.	no

C214	C213	B2	C219	-167.5(4)	.	.	.	.	no
C218	C213	B2	C21	-107.7(5)	.	.	.	.	no
C218	C213	C214	F214	177.5(4)	.	.	.	.	no
C218	C213	C214	C215	-2.2(6)	.	.	.	.	no
B2	C213	C214	F214	-0.3(6)	.	.	.	.	no
B2	C213	C214	C215	180.0(4)	.	.	.	.	no
C214	C213	C218	F218	-176.5(4)	.	.	.	.	no
C214	C213	C218	C217	3.8(6)	.	.	.	.	no
B2	C213	C218	F218	1.1(7)	.	.	.	.	no
B2	C213	C218	C217	-178.6(4)	.	.	.	.	no
C214	C213	B2	C21	69.8(5)	.	.	.	.	no
C214	C213	B2	C27	-53.7(5)	.	.	.	.	no
C218	C213	B2	C219	15.1(7)	.	.	.	.	no
C218	C213	B2	C27	128.8(5)	.	.	.	.	no
C13	C14	C15	C16	4.4(12)	.	.	.	.	no
C13	C14	C15	Ti1	66.5(8)	.	.	.	.	no
F214	C214	C215	F215	0.3(6)	.	.	.	.	no
F214	C214	C215	C216	-179.9(4)	.	.	.	.	no
C213	C214	C215	F215	180.0(4)	.	.	.	.	no
C213	C214	C215	C216	-0.2(7)	.	.	.	.	no
F215	C215	C216	F216	-0.2(7)	.	.	.	.	no
F215	C215	C216	C217	-179.0(4)	.	.	.	.	no
C214	C215	C216	F216	180.0(4)	.	.	.	.	no
C214	C215	C216	C217	1.2(7)	.	.	.	.	no
Ti1	C15	C16	C17	95.1(4)	.	.	.	.	no
C14	C15	C16	Ti1	66.7(6)	.	.	.	.	no
C14	C15	C16	C11	1.1(8)	.	.	.	.	no
C14	C15	C16	C17	161.9(6)	.	.	.	.	no
Ti1	C15	C16	C11	-65.7(4)	.	.	.	.	no
C15	C16	C17	C110	-81.1(5)	.	.	.	.	no
Ti1	C16	C17	C19	-120.4(4)	.	.	.	.	no
F216	C216	C217	F217	1.8(7)	.	.	.	.	no
F216	C216	C217	C218	-178.5(4)	.	.	.	.	no
C215	C216	C217	F217	-179.5(4)	.	.	.	.	no
C215	C216	C217	C218	0.3(7)	.	.	.	.	no
Ti1	C16	C17	C18	117.0(4)	.	.	.	.	no
C11	C16	C17	C19	-40.7(6)	.	.	.	.	no
Ti1	C16	C17	C110	-1.5(3)	.	.	.	.	no
C11	C16	C17	C18	-163.4(5)	.	.	.	.	no
C15	C16	C17	C19	160.1(5)	.	.	.	.	no
C11	C16	C17	C110	78.2(5)	.	.	.	.	no
C15	C16	C17	C18	37.4(7)	.	.	.	.	no
F217	C217	C218	C213	176.8(4)	.	.	.	.	no
F217	C217	C218	F218	-3.0(6)	.	.	.	.	no
C16	C17	C110	Ti1	1.5(3)	.	.	.	.	no
C18	C17	C110	Ti1	-117.4(4)	.	.	.	.	no
C19	C17	C110	Ti1	120.0(4)	.	.	.	.	no
C16	C17	C110	C111	-78.2(5)	.	.	.	.	no
C18	C17	C110	C111	162.9(5)	.	.	.	.	no
C19	C17	C110	C111	40.3(7)	.	.	.	.	no
C16	C17	C110	C114	79.9(5)	.	.	.	.	no
C18	C17	C110	C114	-39.0(7)	.	.	.	.	no
C19	C17	C110	C114	-161.6(5)	.	.	.	.	no
C216	C217	C218	F218	177.3(4)	.	.	.	.	no
C216	C217	C218	C213	-3.0(7)	.	.	.	.	no
C220	C219	C224	C223	0.5(7)	.	.	.	.	no
C220	C219	B2	C21	166.9(4)	.	.	.	.	no
C220	C219	B2	C27	-70.3(5)	.	.	.	.	no
C220	C219	B2	C213	50.4(6)	.	.	.	.	no
C224	C219	B2	C21	-21.6(6)	.	.	.	.	no
C224	C219	B2	C27	101.3(5)	.	.	.	.	no

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 B2      C219    C224    F224        8.1(7)     .      .      .      .   no
 B2      C219    C224    C223     -171.5(4)     .      .      .      .   no
 C224    C219    C220    F220     -178.0(4)     .      .      .      .   no
 C224    C219    C220    C221        1.6(7)     .      .      .      .   no
 B2      C219    C220    F220       -5.4(6)     .      .      .      .   no
 B2      C219    C220    C221      174.1(5)     .      .      .      .   no
 C220    C219    C224    F224     -179.9(4)     .      .      .      .   no
 C224    C219    B2      C213     -138.0(5)     .      .      .      .   no
 F220    C220    C221    C222      176.9(4)     .      .      .      .   no
 F220    C220    C221    F221       -3.1(7)     .      .      .      .   no
 C219    C220    C221    F221      177.3(4)     .      .      .      .   no
 C219    C220    C221    C222       -2.6(8)     .      .      .      .   no
 C220    C221    C222    C223        1.4(8)     .      .      .      .   no
 F221    C221    C222    F222       -0.5(8)     .      .      .      .   no
 F221    C221    C222    C223     -178.5(5)     .      .      .      .   no
 C220    C221    C222    F222      179.5(5)     .      .      .      .   no
 C221    C222    C223    F223      178.7(5)     .      .      .      .   no
 C221    C222    C223    C224        0.5(8)     .      .      .      .   no
 F222    C222    C223    C224     -177.5(4)     .      .      .      .   no
 F222    C222    C223    F223        0.7(7)     .      .      .      .   no
 F223    C223    C224    F224        0.7(6)     .      .      .      .   no
 C222    C223    C224    C219       -1.6(7)     .      .      .      .   no
 F223    C223    C224    C219     -179.7(4)     .      .      .      .   no
 C222    C223    C224    F224      178.8(4)     .      .      .      .   no
 Ti1     C110    C111    C112       66.1(4)     .      .      .      .   no
 C17     C110    C111    Ti1        95.8(4)     .      .      .      .   no
 C17     C110    C111    C112      161.9(5)     .      .      .      .   no
 C114    C110    C111    Ti1       -64.8(4)     .      .      .      .   no
 C114    C110    C111    C112        1.3(6)     .      .      .      .   no
 Ti1     C110    C114    C113       -66.7(4)     .      .      .      .   no
 C17     C110    C114    Ti1        -95.1(4)     .      .      .      .   no
 C17     C110    C114    C113     -161.8(4)     .      .      .      .   no
 C111    C110    C114    Ti1        65.5(4)     .      .      .      .   no
 C111    C110    C114    C113       -1.2(6)     .      .      .      .   no
 Ti1     C111    C112    C113       62.8(4)     .      .      .      .   no
 C110    C111    C112    Ti1       -63.6(4)     .      .      .      .   no
 C110    C111    C112    C113       -0.8(7)     .      .      .      .   no
 Ti1     C112    C113    C114       62.9(3)     .      .      .      .   no
 C111    C112    C113    Ti1       -62.8(4)     .      .      .      .   no
 C111    C112    C113    C114        0.1(6)     .      .      .      .   no
 Ti1     C113    C114    C110       65.6(4)     .      .      .      .   no
 C112    C113    C114    Ti1       -64.9(4)     .      .      .      .   no
 C112    C113    C114    C110        0.7(6)     .      .      .      .   no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 Ti1     H116"        2.6100                    .      .                  no
 Ti1     H13          3.4600                    .      .                  no
 Ti1     H116         2.6100                    .      .                  no
 Ti1     H116'        2.6100                    .      .                  no
 F22     C213       3.097(5)                    .      .                  no
 F22     C219       2.971(5)                    .      .                  no
 F22     C224       3.100(6)                    .      .                  no
 F22     C218       3.170(5)                    .      .                  no
 F22     F23        2.663(3)                    .      .                  no
 F22     F218       2.920(4)                    .      .                  no
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F22	F224	2.910(4)	.	.	no
F23	F221	2.978(4)	.	1_455	no
F23	C14	3.365(7)	.	1_565	no
F23	F22	2.663(3)	.	.	no
F23	F24	2.754(4)	.	.	no
F24	C212	3.347(5)	.	1_455	no
F24	C211	3.345(5)	.	1_455	no
F24	F23	2.754(4)	.	.	no
F24	F25	2.726(4)	.	.	no
F24	F220	2.829(3)	.	1_455	no
F25	F211	2.886(3)	.	1_455	no
F25	C11	3.250(6)	.	.	no
F25	F24	2.726(4)	.	.	no
F25	F26	2.628(3)	.	.	no
F25	C12	3.268(7)	.	.	no
F26	F28	2.755(4)	.	.	no
F26	C28	2.799(5)	.	.	no
F26	F25	2.628(3)	.	.	no
F26	F214	2.864(4)	.	.	no
F26	C27	2.875(5)	.	.	no
F28	C26	3.012(5)	.	.	no
F28	F26	2.755(4)	.	.	no
F28	C224	3.114(5)	.	.	no
F28	F29	2.670(4)	.	.	no
F28	F224	2.869(4)	.	.	no
F28	C21	2.980(5)	.	.	no
F28	C219	3.148(5)	.	.	no
F28	F29	2.970(4)	.	3_665	no
F29	C28	3.142(5)	.	3_665	no
F29	C223	3.329(5)	.	3_665	no
F29	F28	2.670(4)	.	.	no
F29	F28	2.970(4)	.	3_665	no
F29	F210	2.743(4)	.	.	no
F29	C29	3.243(5)	.	3_665	no
F22	H18'	2.8300	.	1_565	no
F22	H15	2.6400	.	1_565	no
F23	H14	2.6000	.	1_565	no
F24	H113	2.6200	.	2_555	no
F25	H12	2.6400	.	.	no
F25	H11	2.6300	.	.	no
F26	H11	2.7300	.	.	no
F26	H111	2.4900	.	.	no
F26	H19'	2.4900	.	.	no
F210	C223	3.368(6)	.	3_665	no
F210	F223	2.798(4)	.	3_665	no
F210	F211	2.719(5)	.	.	no
F210	F29	2.743(4)	.	.	no
F211	F210	2.719(5)	.	.	no
F211	F212	2.635(4)	.	.	no
F211	F25	2.886(3)	.	1_655	no
F211	F217	2.863(4)	.	2_645	no
F212	F220	2.826(4)	.	.	no
F212	C214	2.785(5)	.	.	no
F212	F214	2.963(3)	.	.	no
F212	C213	2.790(5)	.	.	no
F212	F211	2.635(4)	.	.	no
F212	C113	2.953(7)	.	2_655	no
F212	F217	2.742(4)	.	2_645	no
F214	F212	2.963(3)	.	.	no
F214	C27	2.970(5)	.	.	no
F214	C26	3.078(5)	.	.	no

F214	F215	2.666(4)	.	.	no
F214	C21	3.074(5)	.	.	no
F214	C212	3.117(5)	.	.	no
F214	F26	2.864(4)	.	.	no
F214	F217	2.949(4)	.	2_645	no
F214	C111	3.367(6)	.	.	no
F215	F216	2.731(4)	.	.	no
F215	F214	2.666(4)	.	.	no
F216	F215	2.731(4)	.	.	no
F216	C110	3.308(5)	.	2_655	no
F216	F217	2.740(4)	.	.	no
F217	F211	2.863(4)	.	2_655	no
F217	F214	2.949(4)	.	2_655	no
F217	C211	2.999(6)	.	2_655	no
F217	F216	2.740(4)	.	.	no
F217	C111	3.325(6)	.	2_655	no
F217	F212	2.742(4)	.	2_655	no
F217	F218	2.632(4)	.	.	no
F217	C212	2.957(5)	.	2_655	no
F218	F217	2.632(4)	.	.	no
F218	C220	2.773(6)	.	.	no
F218	F22	2.920(4)	.	.	no
F218	C219	2.872(5)	.	.	no
F218	F220	2.701(4)	.	.	no
F220	F212	2.826(4)	.	.	no
F220	C27	3.154(5)	.	.	no
F220	F24	2.829(3)	.	1_655	no
F220	F221	2.669(4)	.	.	no
F220	F218	2.701(4)	.	.	no
F220	C213	2.947(5)	.	.	no
F220	C218	2.907(5)	.	.	no
F220	C212	3.121(5)	.	.	no
F221	F23	2.978(4)	.	1_655	no
F221	F222	2.730(5)	.	.	no
F221	F220	2.669(4)	.	.	no
F222	F223	2.857(4)	.	3_675	no
F222	F221	2.730(5)	.	.	no
F222	F223	2.734(5)	.	.	no
F223	F222	2.857(4)	.	3_675	no
F223	F210	2.798(4)	.	3_665	no
F223	F224	2.642(4)	.	.	no
F223	F222	2.734(5)	.	.	no
F224	C22	2.828(5)	.	.	no
F224	F28	2.869(4)	.	.	no
F224	C21	2.792(5)	.	.	no
F224	F22	2.910(4)	.	.	no
F224	F223	2.642(4)	.	.	no
F211	H12	2.5000	.	1_655	no
F212	H113	2.4400	.	2_655	no
F214	H111	2.7300	.	.	no
F215	H116"	2.7300	.	2_555	no
F216	H19	2.6800	.	2_655	no
F216	H18"	2.8300	.	2_655	no
F216	H13	2.5700	.	2_555	no
F221	H14	2.6400	.	1_665	no
F222	H19"	2.8600	.	3_665	no
F223	H18	2.7200	.	1_565	no
C11	C14	2.637(9)	.	.	no
C11	C15	2.357(8)	.	.	no
C11	F25	3.250(6)	.	.	no
C11	C110	3.016(7)	.	.	no

C11	C111	3.120(8)	.	.	no
C11	C17	2.570(7)	.	.	no
C11	C115	3.384(8)	.	.	no
C12	F25	3.268(7)	.	.	no
C13	C115	3.403(10)	.	.	no
C13	C116	3.439(10)	.	.	no
C14	F23	3.365(7)	.	1_545	no
C15	C17	2.595(7)	.	.	no
C15	C11	2.357(8)	.	.	no
C15	C116	3.267(8)	.	.	no
C15	C12	2.619(9)	.	.	no
C15	C110	3.069(7)	.	.	no
C15	C114	3.200(8)	.	.	no
C16	C114	3.061(7)	.	.	no
C16	C110	2.310(7)	.	.	no
C16	C14	2.374(8)	.	.	no
C16	C12	2.378(8)	.	.	no
C16	C111	3.045(7)	.	.	no
C18	C222	3.503(8)	.	1_545	no
C18	C223	3.283(7)	.	1_545	no
C19	C29	3.564(7)	.	.	no
C21	F214	3.074(5)	.	.	no
C21	F28	2.980(5)	.	.	no
C21	F224	2.792(5)	.	.	no
C22	F224	2.828(5)	.	.	no
C22	C224	3.395(7)	.	.	no
C26	C28	3.393(6)	.	.	no
C26	F214	3.078(5)	.	.	no
C26	F28	3.012(5)	.	.	no
C27	F214	2.970(5)	.	.	no
C27	F220	3.154(5)	.	.	no
C27	F26	2.875(5)	.	.	no
C28	C26	3.393(6)	.	.	no
C28	F29	3.142(5)	.	3_665	no
C28	F26	2.799(5)	.	.	no
C29	C19	3.564(7)	.	.	no
C29	F29	3.243(5)	.	3_665	no
C110	C11	3.016(7)	.	.	no
C110	F216	3.308(5)	.	2_645	no
C110	C112	2.312(10)	.	.	no
C110	C16	2.310(7)	.	.	no
C110	C15	3.069(7)	.	.	no
C110	C113	2.367(8)	.	.	no
C110	C216	3.542(6)	.	2_645	no
C111	C113	2.365(9)	.	.	no
C111	C114	2.311(8)	.	.	no
C111	C11	3.120(8)	.	.	no
C111	C17	2.600(7)	.	.	no
C111	C16	3.045(7)	.	.	no
C11	H19'	2.7700	.	.	no
C111	F214	3.367(6)	.	.	no
C111	C115	3.356(8)	.	.	no
C11	H111	3.0500	.	.	no
C111	F217	3.325(6)	.	2_645	no
C112	C115	3.007(9)	.	.	no
C12	H115	2.9000	.	.	no
C12	H115'	2.9800	.	.	no
C112	C114	2.409(10)	.	.	no
C112	C110	2.312(10)	.	.	no
C13	H115	3.0900	.	.	no
C113	C110	2.367(8)	.	.	no

C13	H116"	3.0900	.	.	no
C113	C116	3.009(8)	.	.	no
C113	C111	2.365(9)	.	.	no
C113	F212	2.953(7)	.	2_645	no
C114	C116	3.230(8)	.	.	no
C14	H116"	2.7500	.	.	no
C14	H116'	3.0400	.	.	no
C114	C112	2.409(10)	.	.	no
C114	C17	2.600(8)	.	.	no
C114	C111	2.311(8)	.	.	no
C114	C15	3.200(8)	.	.	no
C114	C16	3.061(7)	.	.	no
C115	C116	3.143(8)	.	.	no
C15	H18'	2.8100	.	.	no
C115	C112	3.007(9)	.	.	no
C115	C111	3.356(8)	.	.	no
C115	C11	3.384(8)	.	.	no
C115	C12	3.003(8)	.	.	no
C115	C13	3.403(10)	.	.	no
C16	H11	2.0600	.	.	no
C116	C115	3.143(8)	.	.	no
C116	C14	2.950(10)	.	.	no
C16	H15	2.0700	.	.	no
C116	C114	3.230(8)	.	.	no
C116	C15	3.267(8)	.	.	no
C116	C113	3.009(8)	.	.	no
C116	C13	3.439(10)	.	.	no
C18	H15	2.7300	.	.	no
C18	H114	2.8500	.	.	no
C19	H11	2.7200	.	.	no
C19	H111	2.8400	.	.	no
C110	H114	2.1100	.	.	no
C110	H111	2.0900	.	.	no
C111	H112	2.1000	.	.	no
C211	F217	2.999(6)	.	2_645	no
C111	H19'	2.6900	.	.	no
C211	F24	3.345(5)	.	1_655	no
C111	H11	3.0100	.	.	no
C212	F217	2.957(5)	.	2_645	no
C112	H113	2.2700	.	.	no
C212	F24	3.347(5)	.	1_655	no
C212	C214	3.350(6)	.	.	no
C112	H111	2.0700	.	.	no
C112	H115"	2.8400	.	.	no
C212	F214	3.117(5)	.	.	no
C212	F220	3.121(5)	.	.	no
C113	H116	2.8500	.	.	no
C113	H112	2.2500	.	.	no
C113	H114	2.2200	.	.	no
C213	F22	3.097(5)	.	.	no
C213	F212	2.790(5)	.	.	no
C213	F220	2.947(5)	.	.	no
C114	H18'	2.6500	.	.	no
C114	H116'	3.0400	.	.	no
C214	C212	3.350(6)	.	.	no
C214	F212	2.785(5)	.	.	no
C114	H113	2.2400	.	.	no
C115	H12	2.9400	.	.	no
C115	H112	2.9700	.	.	no
C216	C110	3.542(6)	.	2_655	no
C116	H14	2.8700	.	.	no

C116	H113	2.9900	.	.	no
C218	F220	2.907(5)	.	.	no
C218	F22	3.170(5)	.	.	no
C218	C220	3.330(7)	.	.	no
C219	F28	3.148(5)	.	.	no
C219	F22	2.971(5)	.	.	no
C219	F218	2.872(5)	.	.	no
C220	F218	2.773(6)	.	.	no
C220	C218	3.330(7)	.	.	no
C222	C18	3.503(8)	.	1_565	no
C223	C18	3.283(7)	.	1_565	no
C223	F210	3.368(6)	.	3_665	no
C223	F29	3.329(5)	.	3_665	no
C224	C22	3.395(7)	.	.	no
C224	F22	3.100(6)	.	.	no
C224	F28	3.114(5)	.	.	no
C210	H19	3.0800	.	.	no
C215	H116"	2.9700	.	2_555	no
C222	H18"	3.0700	.	1_565	no
C223	H18	2.8000	.	1_565	no
H115'	C12	2.9800	.	.	no
H115"	H112	2.5800	.	.	no
H116'	Ti1	2.6100	.	.	no
H116'	C14	3.0400	.	.	no
H116'	C114	3.0400	.	.	no
H116"	Ti1	2.6100	.	.	no
H116"	C13	3.0900	.	.	no
H116"	C14	2.7500	.	.	no
H116"	H14	2.4900	.	.	no
H116"	F215	2.7300	.	2_545	no
H116"	C215	2.9700	.	2_545	no
H11	F25	2.6300	.	.	no
H11	F26	2.7300	.	.	no
H11	C19	2.7200	.	.	no
H11	H19'	2.2100	.	.	no
H12	F25	2.6400	.	.	no
H12	F211	2.5000	.	1_455	no
H12	C115	2.9400	.	.	no
H13	Ti1	3.4600	.	.	no
H13	F216	2.5700	.	2_545	no
H14	F23	2.6000	.	1_545	no
H14	F221	2.6400	.	1_445	no
H14	C116	2.8700	.	.	no
H14	H116"	2.4900	.	.	no
H15	F22	2.6400	.	1_545	no
H15	C18	2.7300	.	.	no
H15	H18'	2.2600	.	.	no
H18	F223	2.7200	.	1_545	no
H18	C223	2.8000	.	1_545	no
H18	H19"	2.6000	.	.	no
H18'	F22	2.8300	.	1_545	no
H18'	C15	2.8100	.	.	no
H18'	C114	2.6500	.	.	no
H18'	H15	2.2600	.	.	no
H18'	H114	2.1900	.	.	no
H18"	C222	3.0700	.	1_545	no
H18"	H19	2.3200	.	.	no
H18"	F216	2.8300	.	2_645	no
H19	C210	3.0800	.	.	no
H19	H18"	2.3200	.	.	no
H19	F216	2.6800	.	2_645	no

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 H19'    F26          2.4900                    .       .                 no
 H19'    C11          2.7700                    .       .                 no
 H19'    C111         2.6900                    .       .                 no
 H19'    H11          2.2100                    .       .                 no
 H19'    H111         2.2000                    .       .                 no
 H19"    H18          2.6000                    .       .                 no
 H19"    F222         2.8600                    .     3_665               no
 H111    F26          2.4900                    .       .                 no
 H111    F214         2.7300                    .       .                 no
 H111    C19          2.8400                    .       .                 no
 H111    H19'         2.2000                    .       .                 no
 H112    H115"        2.5800                    .       .                 no
 H113    H116         2.5800                    .       .                 no
 H113    F24          2.6200                    .     2_545               no
 H113    F212         2.4400                    .     2_645               no
 H114    C18          2.8500                    .       .                 no
 H114    H18'         2.1900                    .       .                 no
 H115    C12          2.9000                    .       .                 no
 H115    C13          3.0900                    .       .                 no
 H116    Ti1          2.6100                    .       .                 no
 H116    C113         2.8500                    .       .                 no
 H116    H113         2.5800                    .       .                 no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C12     H12     F211        0.9500     2.5000   3.409(7)     161.00   1_455 yes
C19     H19'    F26         0.9800     2.4900   3.472(6)     175.00     .   yes
C111    H111    F26         0.9500     2.4900   3.421(6)     166.00     .   yes
C113    H113    F212        0.9500     2.4400   2.953(7)     114.00   2_645 yes

#===END of Crystallographic Information File
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